Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 7200 L/kg

Global applicability domain: Outside

Local applicability domain index: 2.73e-01

Confidence level: 5.18e-01

Nearest Neighbors from the Training Set

Image not found
Di(2-ethylhexyl) adipate
Measured: 15500
Predicted: 14400

Image not found
Dioctyl phthalate
Measured: 24000
Predicted: 17100

Image not found
Dihexyl phthalate
Measured: 52500
Predicted: 23600

Image not found
2,4-DB 2-butoxyethyl ester
Measured: 501
Predicted: 1980